IUCLID

Data Set

Existing Chemical	:	ID: 4083-64-1
CAS No.	:	4083-64-1
EINECS Name	:	p-toluenesulphonyl isocyanate
EC No.	:	223-810-8
Molecular Formula	:	C8H7NO3S

Producer related part

Company	:	Epona Associates, LLC
Creation date	:	09.06.2003

Substance related part

Company	:	Epona Associates, LLC
Creation date	:	09.06.2003
Status	:	
Memo	:	ISOCHEM Inc.
Printing date	:	12.12.2006
Revision date	:	
Date of last update	:	12.12.2006
Number of pages	:	29
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	typical for marketed substance
Substance type	:	organic
Physical status	:	liquid
Purity	:	>= 98 % w/w
Colour	:	
Odour	:	acrid
Remark	:	PTSI reacts rapidly with excess water to form the corresponding carbamic acid, which in turn, undergoes immediate decomposition to form carbon dioxide and p-toluenesulfonamide (PTSA; CAS number 70-55-3). PTSI is not likely to be found in the environment. Biodegradation, acute aquatic toxicity, repeated dose toxicity, in vitro bacterial mutagenicity and mammalian cytogenicity, reproduction and developmental effects studies are provided for PTSA as supporting data for describing the toxicity of PTSI.
Reliability	:	(1) valid without restriction

12.12.2006 (20)

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

4-Methylbenzenesulfonyl isocyanate

12.12.2006 (1)

4-Methylphenylsulfonyl isocyanate

02.04.2004 (1)

4-Toluenesulfonyl isocyanate

02.04.2004 (1)

Benzenesulfonyl isocyanate, 4-methyl-

12.12.2006 (1)

p-Toluenesulfonic acid, anhydride with isocyanic acid

02.04.2004 (1)

p-Toluenesulfonyl isocyanate

12.12.2006 (1)

p-Tolylsulfonyl isocyanate

02.04.2004 (1)

p-Tosyl isocyanate

02.04.2004 (1)

PTSI

02.04.2004

Sulfone, isocyanato tolyl

02.04.2004 (1)

Tosyl isocyanate

12.12.2006 (1)

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= -2 °C
Sublimation	:	
Method	:	
Year	:	2002
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Freezing Point
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

09.06.2003 (21)

2.2 BOILING POINT

Value	:	= 144 °C at 1333 hPa
Decomposition	:	
Method	:	
Year	:	2002
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Pressure 10 mm Hg
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

01.06.2004 (21)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	.014 hPa at 25 °C
Decomposition	:	
Method	:	OECD Guide-line 104 "Vapour Pressure Curve"
Year	:	2006
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	The vapor pressure was determined using a vapor pressure balance with measurements being made at several temperatures and linear regression analysis used to calculate the vapor pressure at 25C.
Reliability	:	(1) valid without restriction Guideline study
Flag	:	Critical study for SIDS endpoint

12.12.2006 (18)

Value	:	= 1.33 hPa at 100 °C
Decomposition	:	
Method	:	
Year	:	2002

GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Result	:	1 mm Hg @ 100 deg C
Reliability	:	(2) valid with restrictions

12.12.2006 (21)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= .82 at °C
pH value	:	
Method	:	
Year	:	1979
GLP	:	no data
Test substance	:	other TS
Test substance	:	CAS Registry Number: 70-55-3 Chemical Name: P-TOLUENESULFONAMIDE Synonyms: 4-METHYLBENZENESULFONAMIDE Molecular Formula: C7H9NO2S Molecular Weight: 171.22
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

02.04.2004 (10)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	= 1318 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	no
Deg. product	:	
Method	:	other: estimated
Year	:	2004
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Deg. products	:	70-55-3 200-741-1 toluene-4-sulphonamide
Result	:	WSKOW v1.41 Results Log Kow (estimated) : 2.34 Log Kow (experimental): not available from database Log Kow used by Water solubility estimates: 2.34 Equation Used to Make Water Sol estimate: Log S (mol/L) = 0.693-0.96 log Kow-0.0092(Tm-25)-0.00314 MW + Correction Melting Pt (Tm) = -2.00 deg C (Use Tm = 25 for all liquids) Correction(s): Value ---------- ----- No Applicable Correction Factors

Log Water Solubility (in moles/L) : -2.175
Water Solubility at 25 deg C (mg/L): 1318

Test condition : log Kow used: 2.34 (estimated)
no-melting pt equation used

Reliability : (2) valid with restrictions
Modeled data

Flag : Critical study for SIDS endpoint

02.04.2004 (9)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
DIRECT PHOTOLYSIS		
Halflife t1/2	:	ca. 8.8 day(s)
Degradation	:	% after
Quantum yield	:	
INDIRECT PHOTOLYSIS		
Sensitizer	:	
Conc. of sensitizer	:	
Rate constant	:	= .00000000000122 cm^3/(molecule*sec)
Degradation	:	% after
Deg. product	:	not measured
Method	:	other (calculated)
Year	:	2004
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4

Result :

SUMMARY (AOP v1.91): HYDROXYL RADICALS
Hydrogen Abstraction = 0.1360 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings = 1.0883 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 1.2243 E-12 cm3/molecule-sec
HALF-LIFE = 8.737 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 104.839 Hrs
** Designates Estimation(s) Using ASSUMED Value(s)

SUMMARY (AOP v1.91): OZONE REACTION

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Test substance	:	SMILES : O=C=NS(=O)(=O)c(ccc(c1)C)c1 CHEM : Benzenesulfonyl isocyanate, 4-methyl- MOL FOR: C8 H7 N1 O3 S1 MOL WT : 197.21
Reliability	:	(2) valid with restrictions Modeled data
Flag	:	Critical study for SIDS endpoint

12.12.2006 (5)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	< 10 minute(s) at 25 °C
t1/2 pH7	:	< 10 minute(s) at 25 °C
t1/2 pH9	:	< 10 minute(s) at 25 °C
Deg. product	:	
Method	:	other
Year	:	2004

GLP : no
Test substance : as prescribed by 1.1 - 1.4
Deg. products : 70-55-3 200-741-1 toluene-4-sulphonamide

Remark : A hydrolysis study has not been conducted on this substance due to safety reasons. PTSI reacts spontaneously and violently with water. Water should not be poured into a vessel containing this substance. Reaction with water results in the production of CO2, and reaction vessels must be vented to avoid pressure build up.

Result : HYDROWIN Program (v1.67) Results:
==========
Compound has an ISOCYANATE group; C=O located at SMILES atom #: 2

***** CALCULATION NOT PERFORMED *****

Even at low pH, the hydrolysis rate is very fast: t1/2 < 10 minutes.

Test substance : SMILES : O=C=NS(=O)(=O)c(ccc(c1)C)c1
CHEM : Benzenesulfonyl isocyanate, 4-methyl-
MOL FOR: C8 H7 N1 O3 S1
MOL WT : 197.21

Reliability : (2) valid with restrictions
Modeled data

Flag : Critical study for SIDS endpoint

12.12.2006 (7)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media :
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: estimated
Year : 2004

Result : Level III Fugacity Model (Full-Output):
==========
Chem Name : Benzenesulfonyl isocyanate, 4-methyl-
Molecular Wt: 197.21
Henry's LC : 5.69e-005 atm-m3/mole (Henrywin program)
Vapor Press : 5.29 mm Hg (Mpbpwin program)
Log Kow : 2.34 (Kowwin program)
Soil Koc : 89.7 (calc by model)

Mass Amount Half-Life Emissions

(percent) (hr) (kg/hr)
Air 6.04 210 1000
Water 31.3 900 1000
Soil 62.5 900 1000
Sediment 0.174 3.6e+003 0

Fugacity Reaction Advection Reaction Advection
(atm) (kg/hr) (kg/hr) (percent) (percent)
Air 1.22e-010 326 986 10.9 32.9
Water 7.36e-010 393 510 13.1 17
Soil 6.66e-009 785 0 26.2 0
Sediment 6.5e-010 0.547 0.0568 0.0182 0.00189

Persistence Time: 544 hr
Reaction Time: 1.08e+003 hr
Advection Time: 1.09e+003 hr
Percent Reacted: 50.1
Percent Advected: 49.9

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 209.7
Water: 900
Soil: 900
Sediment: 3600
Biowin estimate: 2.689 (weeks-months)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

Test substance : Chem Name : Benzenesulfonyl isocyanate, 4-methyl-
Molecular Wt: 197.21
Reliability : (2) valid with restrictions
Modeled data
Flag : Critical study for SIDS endpoint
12.12.2006 (8)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge
Concentration : 100 mg/l related to Test substance
related to

Contact time	:	28 day(s)
Degradation	:	(±) % after
Result	:	other: not readily biodegradable
Deg. product	:	
Method	:	OECD Guide-line 301 C "Ready Biodegradability: Modified MITI Test (I)"
Year	:	
GLP	:	no
Test substance	:	other TS

Method : The sludge samples were mixed by stirring in a single container and cultured at 25C for 1 month.

Remark : Additional details were not available at http://www.chem.unep.ch/irptc/sids/oecdsids/70553.pdf

Result : 1% Degree of biodegradation from BOD7
4% Degree of biodegradation from BOD14
3% Degree of biodegradation from BOD28
0% Degree of biodegradation from DOC
0% Degree of biodegradation from HPLC

Test substance : Benzenesulfonamide, 4-methyl- CAS 70-55-3: 97.4% pure

Reliability : (2) valid with restrictions
Guideline study but not GLP

Flag : Critical study for SIDS endpoint

12.12.2006 (15) (16)

Type	:	anaerobic
Inoculum	:	Pseudomonas sp. (Bacteria)
Contact time	:	
Degradation	:	(±) % after
Result	:	other: low biodegradability
Deg. product	:	
Method	:	
Year	:	2001
GLP	:	no data
Test substance	:	other TS

Result : A bacterium capable of utilising p-toluenesulphonamide was isolated from activated sludge. The isolated strain designated PTSA was identified as a Pseudomonas sp. using chemotaxonomic and genetic studies. Pseudomonas PTSA grew on p-toluenesulphonamide in a chemostat with approximately 90% release of sulphate and 80% release of ammonium. The isolate was also able to grow on 4-carboxybenzenesulphonamide and 3,4-dihydroxybenzoate but did not grow on p-toluenesulphonate. The transient appearance of

4-hydroxymethylbenzenesulphonamide and 4-carboxybenzenesulphonamide during p-toluenesulphonamide degradation proves oxidation of the methyl group is the initial attack in the biodegradation pathway. Both metabolites of p-toluenesulphonamide degradation were identified by high-performance liquid chromatography-mass spectrometry. 4-Carboxybenzenesulphonamide is probably converted into 3,4-dihydroxybenzoate and amidosulphurous acid. The latter is a chemically unstable compound in aqueous

solutions and
immediately converted into sulphite and ammonium. Both sulphite and
ammonium were formed during degradation of 4-carboxybenzenesulphonamide.

Test substance : CAS Registry Number: 70-55-3
Chemical Name: P-TOLUENESULFONAMIDE
Synonyms: 4-METHYLBENZENESULFONAMIDE
Molecular Formula: C7H9NO2S
Molecular Weight: 171.22

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
12.12.2006 (19)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	semistatic
Species	:	Oryzias latipes (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	435
LC100	:	583
LC0	:	324
Method	:	other: OECD TG not specified
Year	:	
GLP	:	no
Test substance	:	other TS
Remark	:	Additional details were not available at http://www.chem.unep.ch/irptc/sids/oecdsids/70553.pdf Summary indicated the study was conducted according to an OECD guideline, but the TG was not specified
Result	:	LC0 for 24, 48, 72 and 96 hours = 324 mg/L (w/v). (Reported as ppm (w/v)). LC50 for 24, 48, 72 and 96 hours = 435 mg/L. LC100 for 24, 48, 72 and 96 hours = 583 mg/L (w/v). (Reported as ppm (w/v)).
Test substance	:	Benzenesulfonamide, 4-methyl- CAS 70-55-3: >98% pure
Reliability	:	(2) valid with restrictions Guideline study but not GLP
Flag	:	Critical study for SIDS endpoint

12.12.2006 (4) (16)

Type	:	flow through
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	60 day(s)
Unit	:	mg/l
Effect Conc	:	= 9
Method	:	other
Year	:	1996
GLP	:	no data
Test substance	:	other TS
Result	:	Effect Endpoint Type: Effect Code (EFF) : GPHY - physiology, general Trend (TREND) : CHG - change Effect Category (EFFCAT): PHY - physiological: change in the organic processes or functions of an organism Effect Tissue (TISSUE): BL - blood
Test condition	:	Age/Life Stage: ADULT, 206.5-670.7 G (grams) Exposure Regimen: 60 (test duration); NR - not reported (minimum duration); NR - not reported (maximum duration); Units: MI - minutes Controls: M - multiple types of controls were reported by the author
Test substance	:	CAS Registry Number: 70-55-3 Chemical Name: P-TOLUENESULFONAMIDE Synonyms: 4-METHYLBENZENESULFONAMIDE Molecular Formula: C7H9NO2S

Molecular Weight: 171.22

Reliability : (2) valid with restrictions
12.12.2006 (17)

Type :
Species :
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : = 1314
LC50 (14-day) : = 2005
Method : other: estimated
Year : 2004
GLP : no
Test substance : other TS

Result : ECOSAR v0.99g Class(es) Found

Neutral Organics

ECOSAR Class	Organism	Duration	Predicted End Pt	mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	Fish	14-day	LC50	2005.498
Neutral Organics	Fish	96-hr	LC50	1314.445

Test condition : MOL FOR: C7 H9 N1 O2 S1
MOL WT : 171.22
Log Kow: 0.92 (KowWin estimate)
Melt Pt:
Wat Sol: 9619 mg/L (calculated)

Test substance : SMILES : O=S(=O)(N)c(ccc(c1)C)c1
CHEM : Benzenesulfonamide, 4-methyl-

Reliability : (2) valid with restrictions
Modeled data
12.12.2006 (6)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : other: not specified
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
EC0 : 32
EC50 : 150
EC100 : 320
Method : other: OECD TG not specified
Year :
GLP : no
Test substance : other TS

Method : Probit method
Remark : Additional details were not available at http://www.chem.unep.ch/irptc/sids/oecdsids/70553.pdf

Result :
EC0 for 24 hours = 32 mg/L (w/v). (Reported as ppm (w/v)).

EC50 for 24 hours = 150 mg/L (w/v). (Reported as ppm (w/v)).

EC100 for 24 hours = 320 mg/L (w/v). (Reported as ppm (w/v)).

Reliability : (2) valid with restrictions
Guideline study but not GLP

Flag : Critical study for SIDS endpoint

12.12.2006 (3) (16)

Type : other
Species : other: Daphnia
Exposure period :
Unit :
Method : other: estimated
Year : 2004
GLP : no
Test substance : other TS

Result : ECOSAR v0.99g Class(es) Found

Neutral Organics

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organics:	Daphnid	48-hr	LC50	1307.201
Neutral Organics:	Daphnid	16-day	EC50	41.797

Test condition : MOL FOR: C7 H9 N1 O2 S1
MOL WT : 171.22
Log Kow: 0.92 (KowWin estimate)
Melt Pt:
Wat Sol: 9619 mg/L (calculated)

Test substance : SMILES : O=S(=O)(N)c(ccc(c1)C)c1
CHEM : Benzenesulfonamide, 4-methyl-

Reliability : (2) valid with restrictions
Modeled data

12.12.2006 (6)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : Selenastrum capricornutum (Algae)
Endpoint :
Exposure period : 72 hour(s)
Unit : mg/l
EC50 : 23
Method : other: OECD TG not specified
Year :
GLP : no
Test substance : other TS

Remark : Additional details were not available at http://www.chem.unep.ch/irptc/sids/oecdsids/70553.pdf

Result : EC50 for 72 hours = 23 mg/L (w/v). (Reported as EbC50 ppm (w/v)).
Activity rises very sharply.

Test substance : Benzenesulfonamide, 4-methyl- CAS 70-55-3: >99% pure
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint

12.12.2006 (2) (16)

Species : other algae: Green algae

Endpoint	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l
EC50	:	= 767
Method	:	other: estimated
Year	:	2004
GLP	:	no
Test substance	:	other TS

Result : ECOSAR v0.99g Class(es) Found

Neutral Organics

ECOSAR

Class	Organism	Duration	End Pt	mg/L (ppm)
Neutral Organics	Green Algae	96-hr	EC50	767.966
Neutral Organics	Green Algae	96-hr	ChV	41.140

Test condition : MOL FOR: C7 H9 N1 O2 S1
MOL WT : 171.22
Log Kow: 0.92 (KowWin estimate)
Melt Pt:
Wat Sol: 9619 mg/L (calculated)

Test substance : SMILES : O=S(=O)(N)c(ccc(c1)C)c1
CHEM : Benzenesulfonamide, 4-methyl-

Reliability : (2) valid with restrictions
Modeled data

12.12.2006 (6)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

12.12.2006

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 2600 mg/kg bw
Species	:	
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Method	:	
Year	:	2002
GLP	:	no data
Test substance	:	as prescribed by 1.1 - 1.4
Reliability	:	(2) valid with restrictions Provides basic data
Flag	:	Critical study for SIDS endpoint

12.12.2006 (21)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type	:	Sub-acute
Species	:	rat
Sex	:	male/female
Strain	:	other: Crj:CD(SD)
Route of admin.	:	gavage
Exposure period	:	42 d prior to mating (M) or 14 d before mating through d 3 lactation (F)
Frequency of treatm.	:	daily
Post exposure period	:	
Doses	:	0, 120, 300, and 750 mg/kg
Control group	:	yes
Method	:	other: OECD 422

Year	:	1994
GLP	:	yes
Test substance	:	other TS
Method	:	Doses of: 0, 120, 300, 750 mg/kg/day were administered by oral gavage for 42 days to groups of 13 male rats and from day 14 before mating through day 3 of lactation to groups of 13 female rats.
Result	:	4 animals from the high-dose groups displayed hematuria within the first 3 days of dosing. Body weights of the high-dose males were significantly lower than the controls throughout the dosing period. A reduction in body weight gain was observed in the mid- and high-dose females during the gestation and/or lactation period. Relative kidney and liver weights were slightly increased in the high-dose animals. In addition dark-colored livers were observed in the 6 high-dose males. In the histopathological examinations urinary bladder epithelium were seen in 6 low and 11 each in mid- and high- dose males and 1 low-, 12 mid- and 7 high-dose females. Haematological examinations indicated a dose dependent increase in white blood cells counts in the mid- and high- dose males. There was also increased number of neutrophils in the high-dose males. BLOOD BIOCH Levels of BUN, GOT and chloride were significantly elevated in the mid- and high-dose males. GPT level was significantly increased and potassium decreased in the high-dose males No adverse effect level was established as 120 mg/kg/day. Estimated dose of low concern was calculated as 0.0240 mg/kg /day under the test conditions. General Comments : A dose dependent increase in the frequency and incidence of hypersalivation was shown in all treated groups. Food consumption of the high-dose males was significantly suppressed in the first week of dosing and in the mid- and high-dose females during the gestation period. There was also observed an involution of the thymus in 8 high- and mid- dose females. Food consumption were recorded at scheduled times during the study. Hematological and blood chemistry measurements and histopathological examinations were done for the males at termination. Pertinent pregnancy and offspring parameters, e.g. (mating performance, duration of gestation, pup viability, body weight and sex distribution, gross anomalies were determined. Dose-related hypersalivation was observed in all treatment groups. Significant decrease in body weight gains in the high-dose Males relative to controls persisted throughout the dosing period. Relative kidney and liver weights were slightly increased in high-dose animals. A dose-dependent increase in white blood cells counts was observed in mid- and high-dose Males and some F (1 low-, 12 mid-, and 7 high-dose groups). An increased number of neutrophils were observed in high-dose M. BUN, GOT, and chloride were significantly elevated in the two highest dose groups (M). GPT levels were significantly elevated and potassium levels decreased in the high-dose Males.

Four animals from the high-dose groups displayed hematuria within the first 3 d of dosing. There was an involution of the thymus in 8 high- and middosed Females.

Test condition : Rat, Crj:CD(SD), adult, age n.p., 13 M and 13 F/dose
Animals dosed orally (0,120, 300, and 750 mg/kg [0, 0.701, 1.75, and 4.38 mmol/kg]) for 42 d prior to mating (M) or 14 d before mating through d 3 lactation (F)

Test substance : p-TSA in 5% gum Arabic solution, >99.9% pure

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

12.12.2006 (11) (12) (16)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Bacterial reverse mutation assay

System of testing : S. typhimurium strains TA98, TA100, TA1535, TA1537; Escherichia coli WP2 ultra violet radiation A

Test concentration : 0, 312.5, 625, 1250, 2500, 5000 µg/plate [1.825, 3.65, 7.300, 14.60, and 29.20 µmol/plate]

Cycotoxic concentr. : 5000 ug/plate

Metabolic activation : with and without

Result : negative

Method : other: Japanese Guideline for Screening Mutagenicity Testing of Chemicals - Plate

Year : 1994

GLP : yes

Test substance : other TS

Method : Postive control: -S9: AF-2 (TA98, TA100), sodium azide (TA1535), 9-aminoacridine (TA1537). +S9: 2-aminoanthracene (all strains). Doses of: 0, 312.5, 625, 1250, 2500, 5000 ug/plate were utilised. 3 plates/test, in 2 replicates.

Result : Mutagenic effects were not observed under the test conditions. Minimum toxic concentration observed for bacteria was 5000 µg/plate [29.20 µmol/plate] with and without activation.

Test substance : p-TSA in DMSO

Reliability : (1) valid without restriction
Guideline study

Flag : Critical study for SIDS endpoint

12.12.2006 (11) (13) (14) (16)

Type : Chromosomal aberration test

System of testing : CHL cells

Test concentration : Without S9: 0, 0.33, 0.65, 1.30 mg/mL [0, 1.93, 3.80, 7.59 mM]; with S9: 0, 0.43, 0.85, 1.70 mg/mL [0, 2.5, 5.0, 9.9 mM].

Cycotoxic concentr. : >2.0 mg/mL [11.68 mM] with metabolic activation and 2.0 mg/mL [11.68 mM] without metabolic activation.

Metabolic activation : with and without

Result : negative

Method : other: Japanese Guideline for Screening Mutagenicity Testing of Chemicals.

Year : 1994

GLP : yes

Test substance : other TS

Method : Positive control: -S9: mitomycin C, +S9: cyclophosphamide. Doses for -S9: 0,
0.33, 0.65, 1.30 mg/mL. Doses for +S9: 0, 0.43, 0.85, 1.70 mg/mL. 2

plates/test.

Result	:	The test material was classified as “negative” for chromosomal aberrations, under the test conditions. The lowest concentration producing cell toxicity was >2.0 mg/mL [11.68 mM] with metabolic activation and 2.0 mg/mL [11.68 mM] without metabolic activation.
Test condition	:	Without S9: 0, 0.33, 0.65, 1.30 mg/mL [0, 1.93, 3.80, 7.59 mM]; with S9: 0, 0.43, 0.85, 1.70 mg/mL [0, 2.5, 5.0, 9.9 mM].
Test substance	:	p-TSA in DMSO, purity 99.9%
Reliability	:	(1) valid without restriction Guideline study
Flag	:	Critical study for SIDS endpoint

12.12.2006 (13) (14) (16)

5.6 GENETIC TOXICITY ‘IN VIVO‘

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

Type	:	One generation study
Species	:	rat
Sex	:	male/female
Strain	:	other: Crj:CD(SD)
Route of admin.	:	gavage
Exposure period	:	42 d prior to mating (M) or 14 d before mating through d 3 lactation (F)
Frequency of treatm.	:	daily
Premating exposure period		
Male	:	42 days
Female	:	14 days
Duration of test	:	
No. of generation studies	:	
Doses	:	0, 120, 300, and 750 mg/kg
Control group	:	yes
NOAEL F1 offspring	:	= 300 mg/kg bw
Method	:	OECD Guide-line 422
Year	:	1994
GLP	:	yes
Test substance	:	other TS
Method	:	Doses of: 0, 120, 300, 750 mg/kg/day were given in oral gavage for 42 days to groups of 13 male rats and from 14 day before mating through day 3 of lactation to groups of 13 female rats.
Result	:	In the high-dose group, newborns showed significant decrease in body weight and survival rate. Two of the high-dose female rats showed signs of difficult labor; all their offspring died by d 3 of lactation. NOAEL for F1 generation was 300 mg/kg [1.75 mmol/kg] under the test conditions. Mating performance and fertility were not affected by the test compound. Reproduction parameters were comparable among all four groups including the control. No remarkable

histopathological changes in the ovaries was observed in any of the non-pregnant females.

No adverse effect level for P generation was 300 mg/kg/day under the test conditions.

Estimated dose of low concern for reproduction was calculated as 0.6 mg/kg/day

Test condition	:	Rat, Crj:CD(SD), adult, 13 M and 13 F/dose Animals dosed orally (0,120, 300, and 750 mg/kg [0, 0.701, 1.75, and 4.38 mmol/kg]) for 42 d prior to mating (M) or 14 d before mating through d 3 lactation (F)
Test substance	:	p-TSA (99.9% pure)
Reliability	:	(1) valid without restriction Guideline study
Flag	:	Critical study for SIDS endpoint

12.12.2006 (11) (12) (16)

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	male/female
Strain	:	other: Crj:CD(SD)
Route of admin.	:	gavage
Exposure period	:	Animals dosed orally for 42 d prior to mating (M) or 14 d before mating through d 3 lactation (F)
Frequency of treatm.	:	daily
Duration of test	:	
Doses	:	0, 120, 300, and 750 mg/kg
Control group	:	yes
NOAEL teratogen.	:	= 300 - mg/kg bw
Method	:	other: OECD 422
Year	:	1994
GLP	:	yes
Test substance	:	other TS
Result	:	Morphological observations for offspring revealed no teratogenic effect of the test substance. NOAEL for F1 generation was 300 mg/kg [1.75 mmol/kg] under the test conditions. The newborns to the high-dose dams showed significant A significant decrease in survival rate was observed in the newborns in the high-dose group. No adverse effect level for F-1 generation was 300 mg/kg under the test conditions. General Comments : Two of the high-dose female rats showed the signs of difficult labor and all of their offspring died by day 3 of lactation. Morphological observation for offspring revealed no teratogenic effect of the test substance.
Test condition	:	Rat, Crj:CD(SD), Maternal doses: 0, 120, 300, 750 mg/kg/d [0, 0.701, 1.75, and 4.38 mmol/kg/d]
Test substance	:	p-TSA (99.9% pure)
Reliability	:	(1) valid without restriction Guideline study
Flag	:	Critical study for SIDS endpoint

12.12.2006 (11) (12) (16)

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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(7) Epiwin (2004) HYDROWIN Program (v1.67)

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(14) MHW (Year not specified) Unpublished Report on Mutagenicity Test conducted by the Ministry of Health and Welfare (MHW), Japan

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT